# Diphenylurea

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102-07-8	DTXSID2025183						

### **Model Performance**

Model	Data

## Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

### **Model Results**

Predicted value: 2.97

Global applicability domain: Inside

Local applicability domain index: 5.26e-01

Confidence level: 6.62e-01

### Nearest Neighbors from the Training Set

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Diphenylurea Measured: 3.00 Predicted: 2.97

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1-(2-chloroethyl)-3-(4-chlorophenyl)-1-nitrosourea

Measured: 3.16 Predicted: 2.43

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2-Anilinophenylacetic acid

Measured: 3.49 Predicted: 3.24